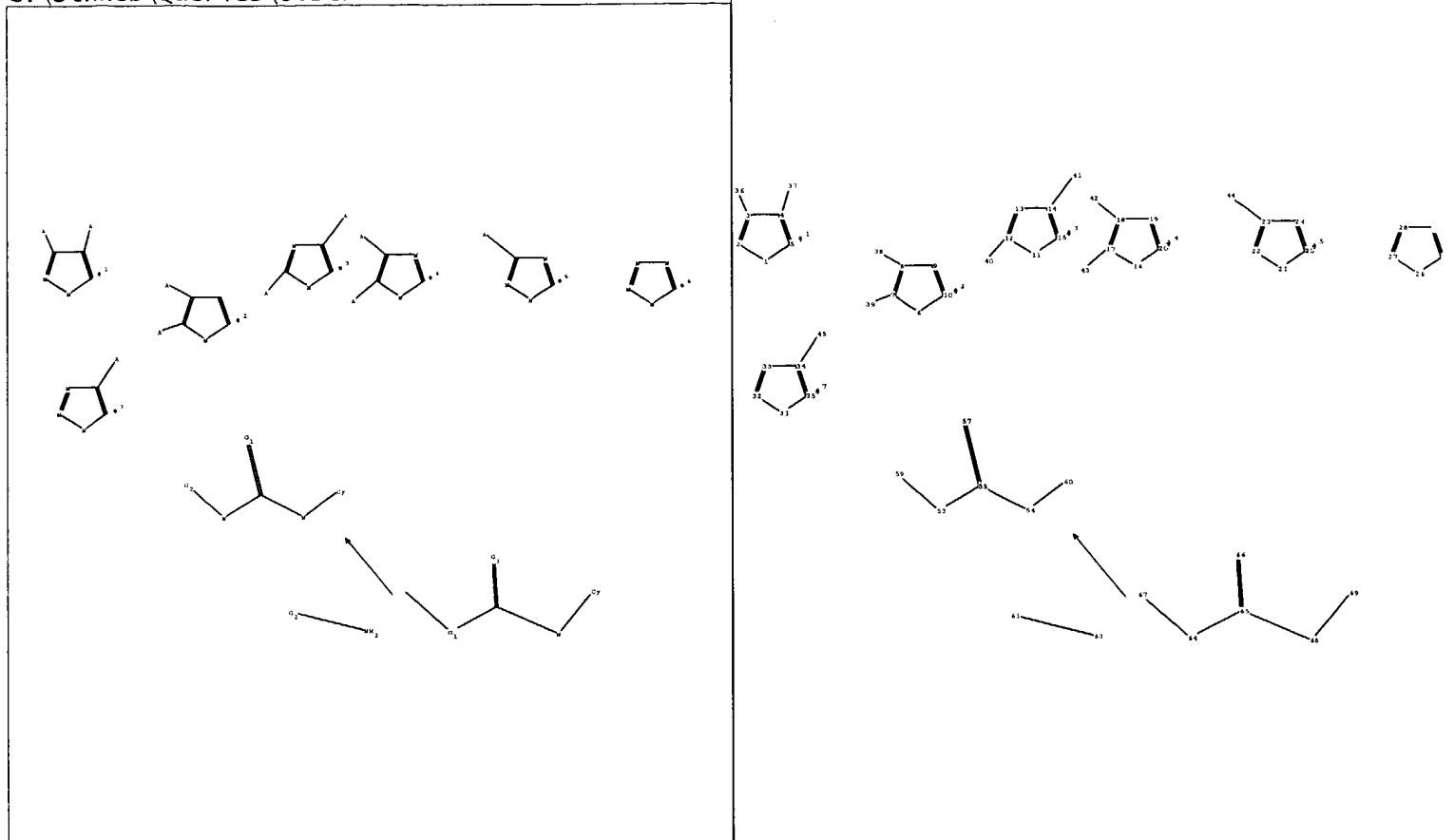


C:\stnweb\Queries\9.str



```

chain nodes :
  38 42 43 53 54 55 57 59 60 61 63 64 65 66 68 69
ring nodes :
  1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16 17 18 19 20 21 22 23 24 25
  26 27 28 29 30 31 32 33 34 35
ring/chain nodes :
  36 37 39 40 41 44 45 67
chain bonds :
  3-36 4-37 7-39 8-38 12-40 14-41 17-43 18-42 23-44 34-45 53-55 53-59 54-55
  54-60 55-57 61-63 64-65 64-67 65-66 65-68 68-69
ring bonds :
  1-2 1-5 2-3 3-4 4-5 6-7 6-10 7-8 8-9 9-10 11-12 11-15 12-13 13-14 14-15
  16-17 16-20 17-18 18-19 19-20 21-22 21-25 22-23 23-24 24-25 26-27 26-30 27-28
  28-29 29-30 31-32 31-35 32-33 33-34 34-35
exact/norm bonds :
  1-2 1-5 2-3 3-4 3-36 4-5 4-37 6-7 6-10 7-8 7-39 8-9 8-38 9-10 11-12 11-15
  12-13 12-40 13-14 14-15 14-41 16-17 16-20 17-18 17-43 18-19 18-42 19-20 21-22
  21-25 22-23 23-24 23-44 24-25 26-27 26-30 27-28 28-29 29-30 31-32 31-35 32-33
  33-34 34-35 34-45 53-55 53-59 54-55 54-60 55-57 61-63 64-65 64-67 65-66 65-68
  68-69

```

G1:O,S

G2:[*1],[*2],[*3],[*4],[*5],[*6],[*7]

Match level :

```

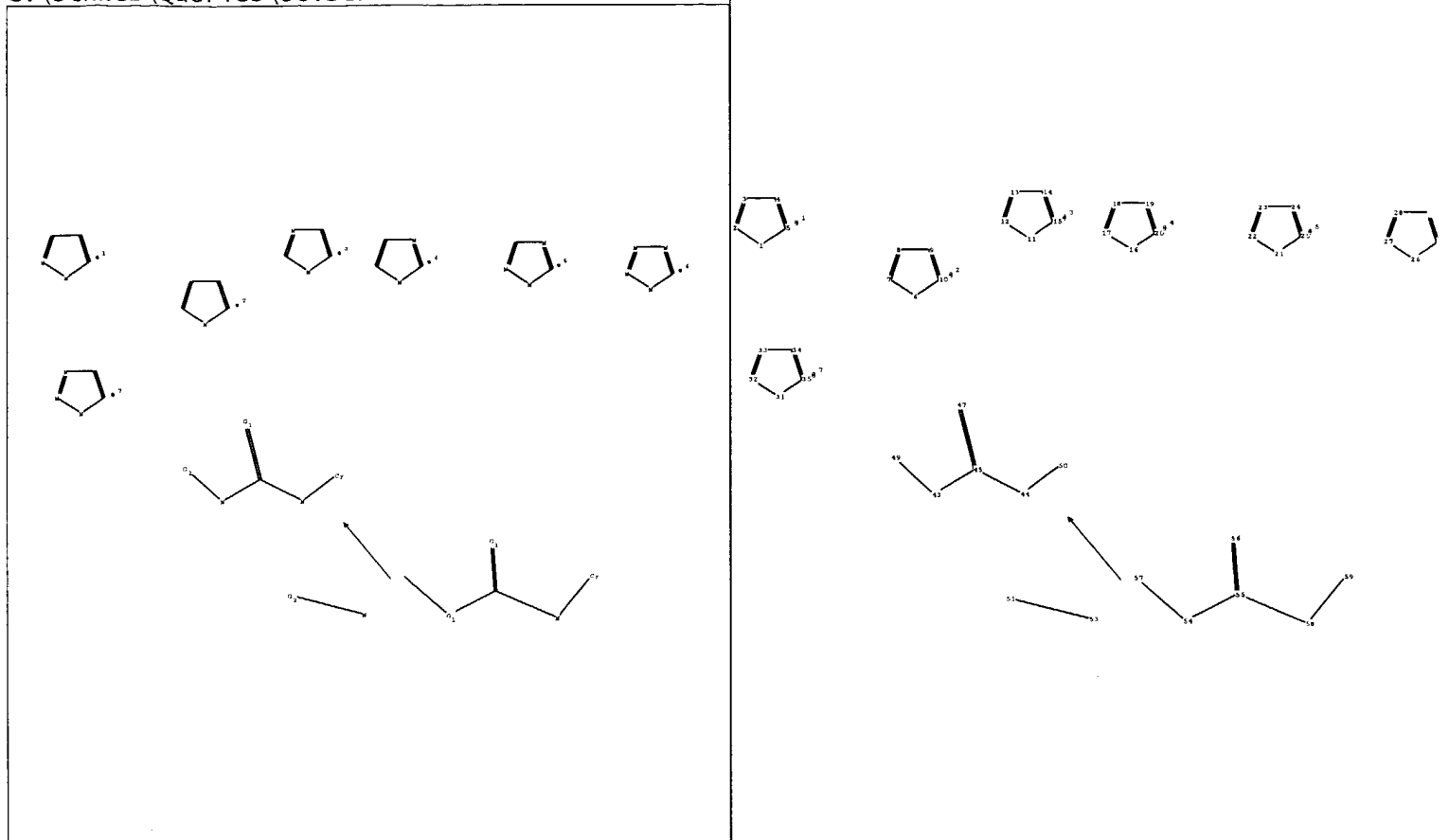
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom 11:Atom
12:Atom 13:Atom 14:Atom 15:Atom 16:Atom 17:Atom 18:Atom 19:Atom 20:Atom 21:Atom
22:Atom 23:Atom 24:Atom 25:Atom 26:Atom 27:Atom 28:Atom 29:Atom 30:Atom 31:Atom
32:Atom 33:Atom 34:Atom 35:Atom 36:CLASS 37:CLASS 38:CLASS 39:CLASS 40:CLASS
41:CLASS 42:CLASS 43:CLASS 44:CLASS 45:CLASS 53:CLASS 54:CLASS 55:CLASS 57:CLASS
59:CLASS 60:Atom 61:CLASS 63:CLASS 64:CLASS 65:CLASS 66:CLASS 67:CLASS 68:CLASS
69:Atom

```

fragments assigned reactant role:

containing 61
containing 64
fragments assigned product role:
containing 53

C:\stnweb\queries\56.str



chain nodes :

43 44 45 47 49 50 51 53 54 55 56 58 59

ring nodes :

1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16 17 18 19 20 21 22 23 24 25
26 27 28 29 30 31 32 33 34 35

ring/chain nodes :

57

chain bonds :

43-45 43-49 44-45 44-50 45-47 51-53 54-55 54-57 55-56 55-58 58-59

ring bonds :

1-2 1-5 2-3 3-4 4-5 6-7 6-10 7-8 8-9 9-10 11-12 11-15 12-13 13-14 14-15
16-17 16-20 17-18 18-19 19-20 21-22 21-25 22-23 23-24 24-25 26-27 26-30 27-28
28-29 29-30 31-32 31-35 32-33 33-34 34-35

exact/norm bonds :

1-2 1-5 2-3 3-4 4-5 6-7 6-10 7-8 8-9 9-10 11-12 11-15 12-13 13-14 14-15
16-17 16-20 17-18 18-19 19-20 21-22 21-25 22-23 23-24 24-25 26-27 26-30 27-28
28-29 29-30 31-32 31-35 32-33 33-34 34-35 43-45 43-49 44-45 44-50 45-47 51-53
54-55 54-57 55-56 55-58 58-59

G1:O,S

G2:[*1],[*2],[*3],[*4],[*5],[*6],[*7]

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom 11:Atom
12:Atom 13:Atom 14:Atom 15:Atom 16:Atom 17:Atom 18:Atom 19:Atom 20:Atom 21:Atom
22:Atom 23:Atom 24:Atom 25:Atom 26:Atom 27:Atom 28:Atom 29:Atom 30:Atom 31:Atom
32:Atom 33:Atom 34:Atom 35:Atom 43:CLASS 44:CLASS 45:CLASS 47:CLASS 49:CLASS
50:Atom 51:CLASS 53:CLASS 54:CLASS 55:CLASS 56:CLASS 57:CLASS 58:CLASS 59:Atom

fragments assigned reactant role:

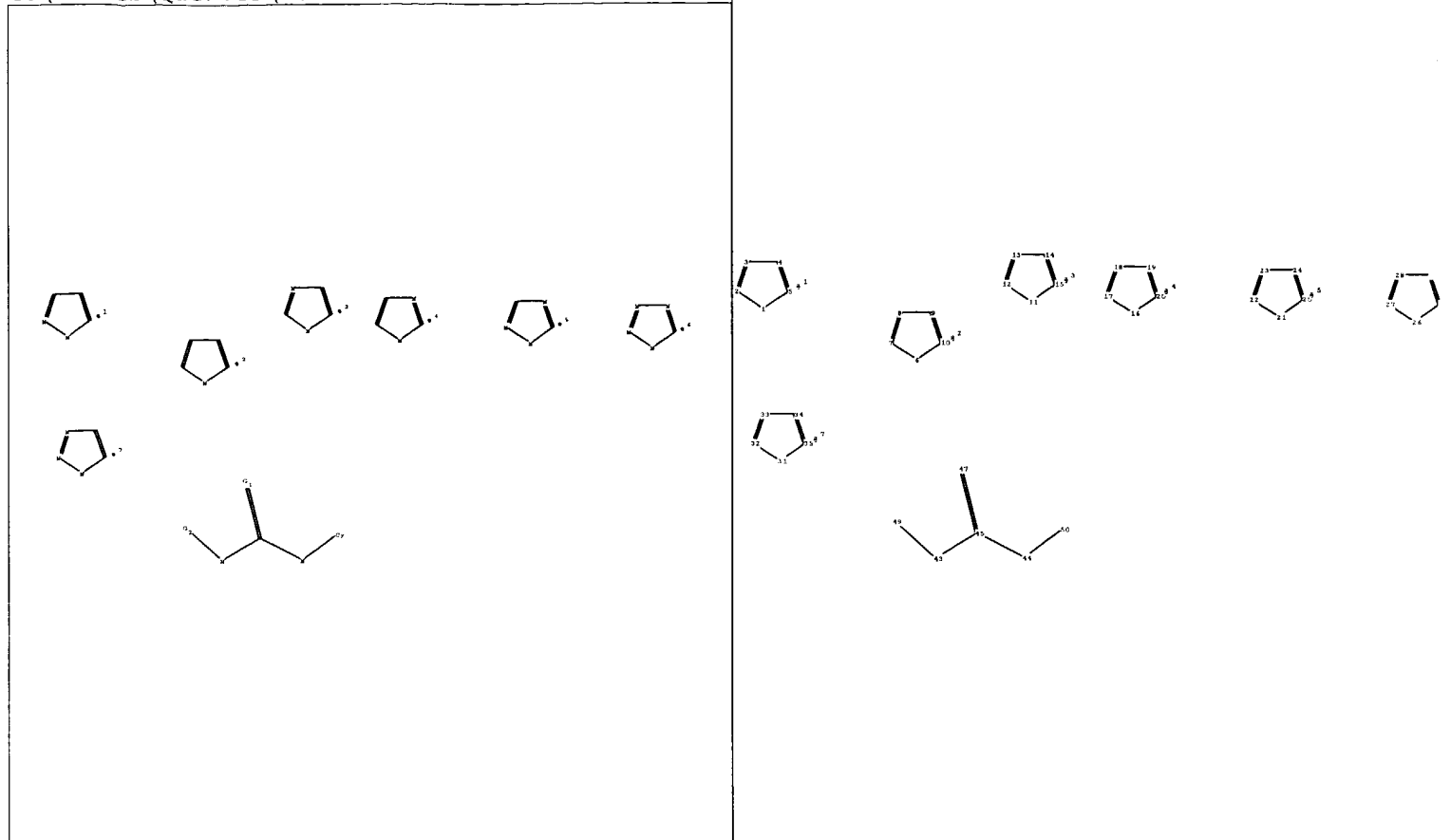
containing 51

containing 54

fragments assigned product role:

containing 43

C:\stnweb\queries\7.str



```

chain nodes :
  43 44 45 47 49 50
ring nodes :
  1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16 17 18 19 20 21 22 23 24 25
  26 27 28 29 30 31 32 33 34 35
chain bonds :
  43-45 43-49 44-45 44-50 45-47
ring bonds :
  1-2 1-5 2-3 3-4 4-5 6-7 6-10 7-8 8-9 9-10 11-12 11-15 12-13 13-14 14-15
  16-17 16-20 17-18 18-19 19-20 21-22 21-25 22-23 23-24 24-25 26-27 26-30 27-28
  28-29 29-30 31-32 31-35 32-33 33-34 34-35
exact/norm bonds :
  1-2 1-5 2-3 3-4 4-5 6-7 6-10 7-8 8-9 9-10 11-12 11-15 12-13 13-14 14-15
  16-17 16-20 17-18 18-19 19-20 21-22 21-25 22-23 23-24 24-25 26-27 26-30 27-28
  28-29 29-30 31-32 31-35 32-33 33-34 34-35 43-45 43-49 44-45 44-50 45-47

```

G1:O,S

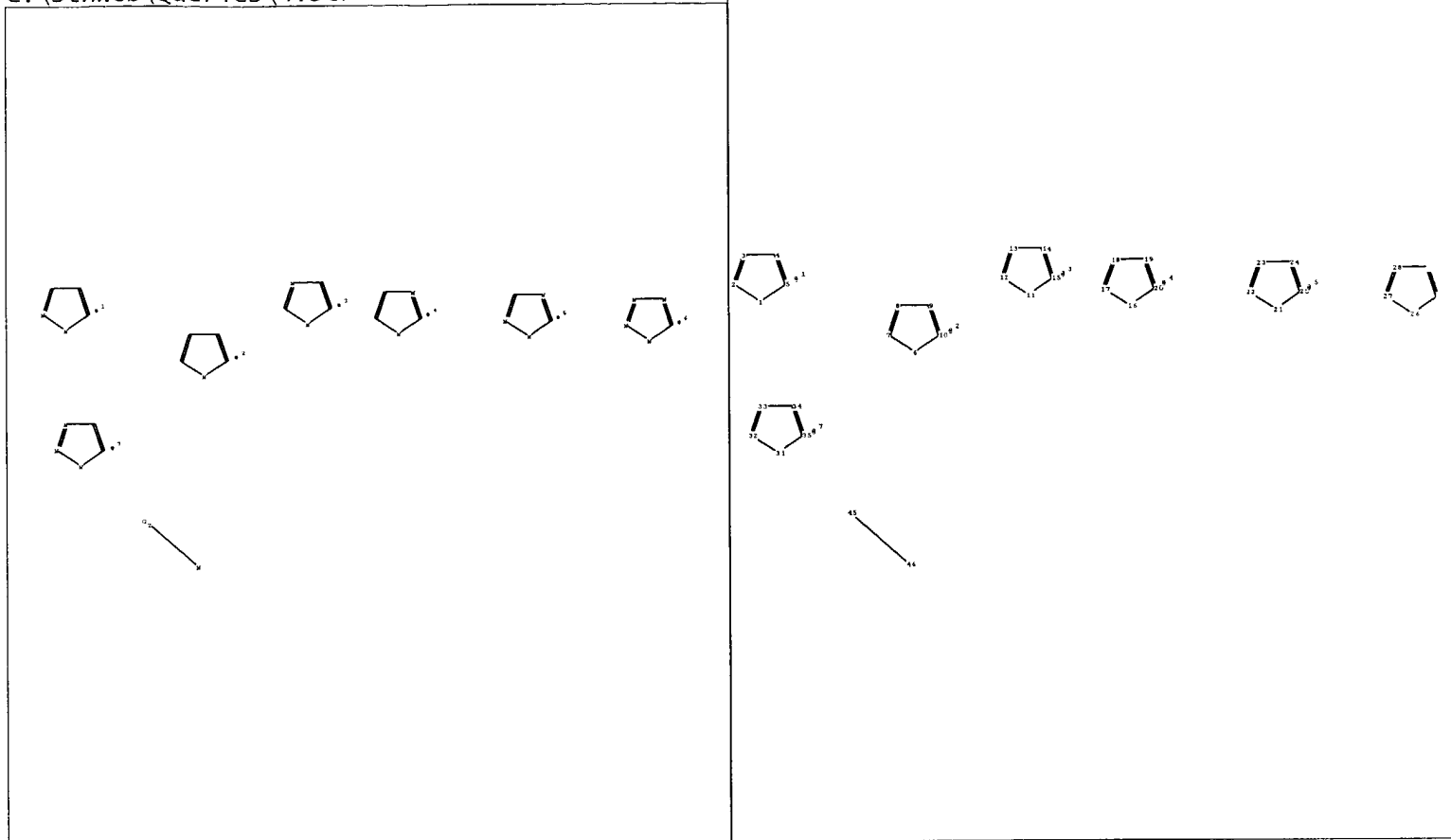
G2:[*1],[*2],[*3],[*4],[*5],[*6],[*7]

```

Match level :
  1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom 11:Atom
  12:Atom 13:Atom 14:Atom 15:Atom 16:Atom 17:Atom 18:Atom 19:Atom 20:Atom 21:Atom
  22:Atom 23:Atom 24:Atom 25:Atom 26:Atom 27:Atom 28:Atom 29:Atom 30:Atom 31:Atom
  32:Atom 33:Atom 34:Atom 35:Atom 43:CLASS 44:CLASS 45:CLASS 47:CLASS 49:CLASS
  50:Atom
fragments assigned product role:
  containing 43

```

c:\stnweb\Queries\4.str



chain nodes :

45 46

ring nodes :

1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16 17 18 19 20 21 22 23 24 25
26 27 28 29 30 31 32 33 34 35

chain bonds :

45-46

ring bonds :

1-2 1-5 2-3 3-4 4-5 6-7 6-10 7-8 8-9 9-10 11-12 11-15 12-13 13-14 14-15
16-17 16-20 17-18 18-19 19-20 21-22 21-25 22-23 23-24 24-25 26-27 26-30 27-28
28-29 29-30 31-32 31-35 32-33 33-34 34-35

exact/norm bonds :

1-2 1-5 2-3 3-4 4-5 6-7 6-10 7-8 8-9 9-10 11-12 11-15 12-13 13-14 14-15
16-17 16-20 17-18 18-19 19-20 21-22 21-25 22-23 23-24 24-25 26-27 26-30 27-28
28-29 29-30 31-32 31-35 32-33 33-34 34-35 45-46

G1:O,S

G2:[*1],[*2],[*3],[*4],[*5],[*6],[*7]

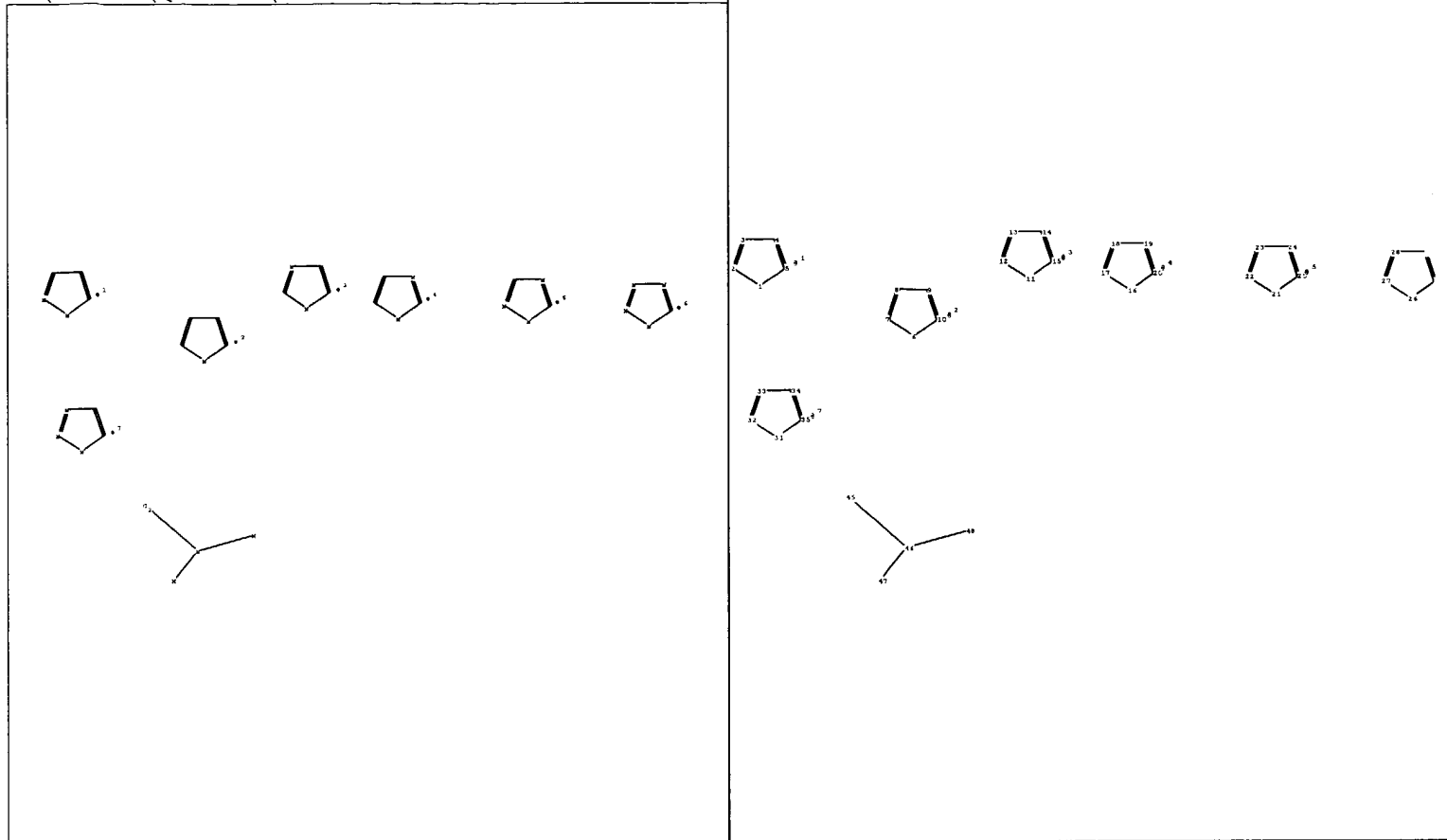
Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom 11:Atom
12:Atom 13:Atom 14:Atom 15:Atom 16:Atom 17:Atom 18:Atom 19:Atom 20:Atom 21:Atom
22:Atom 23:Atom 24:Atom 25:Atom 26:Atom 27:Atom 28:Atom 29:Atom 30:Atom 31:Atom
32:Atom 33:Atom 34:Atom 35:Atom 45:CLASS 46:CLASS

fragments assigned product role:

containing 45

C:\stnweb\Queries\6.str



chain nodes :

45 46 47 48

ring nodes :

1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16 17 18 19 20 21 22 23 24 25
26 27 28 29 30 31 32 33 34 35

chain bonds :

45-46 46-48 46-47

ring bonds :

1-2 1-5 2-3 3-4 4-5 6-7 6-10 7-8 8-9 9-10 11-12 11-15 12-13 13-14 14-15
16-17 16-20 17-18 18-19 19-20 21-22 21-25 22-23 23-24 24-25 26-27 26-30 27-28
28-29 29-30 31-32 31-35 32-33 33-34 34-35

exact/norm bonds :

1-2 1-5 2-3 3-4 4-5 6-7 6-10 7-8 8-9 9-10 11-12 11-15 12-13 13-14 14-15
16-17 16-20 17-18 18-19 19-20 21-22 21-25 22-23 23-24 24-25 26-27 26-30 27-28
28-29 29-30 31-32 31-35 32-33 33-34 34-35 45-46

exact bonds :

46-48 46-47

G1:0,S

G2:[*1],[*2],[*3],[*4],[*5],[*6],[*7]

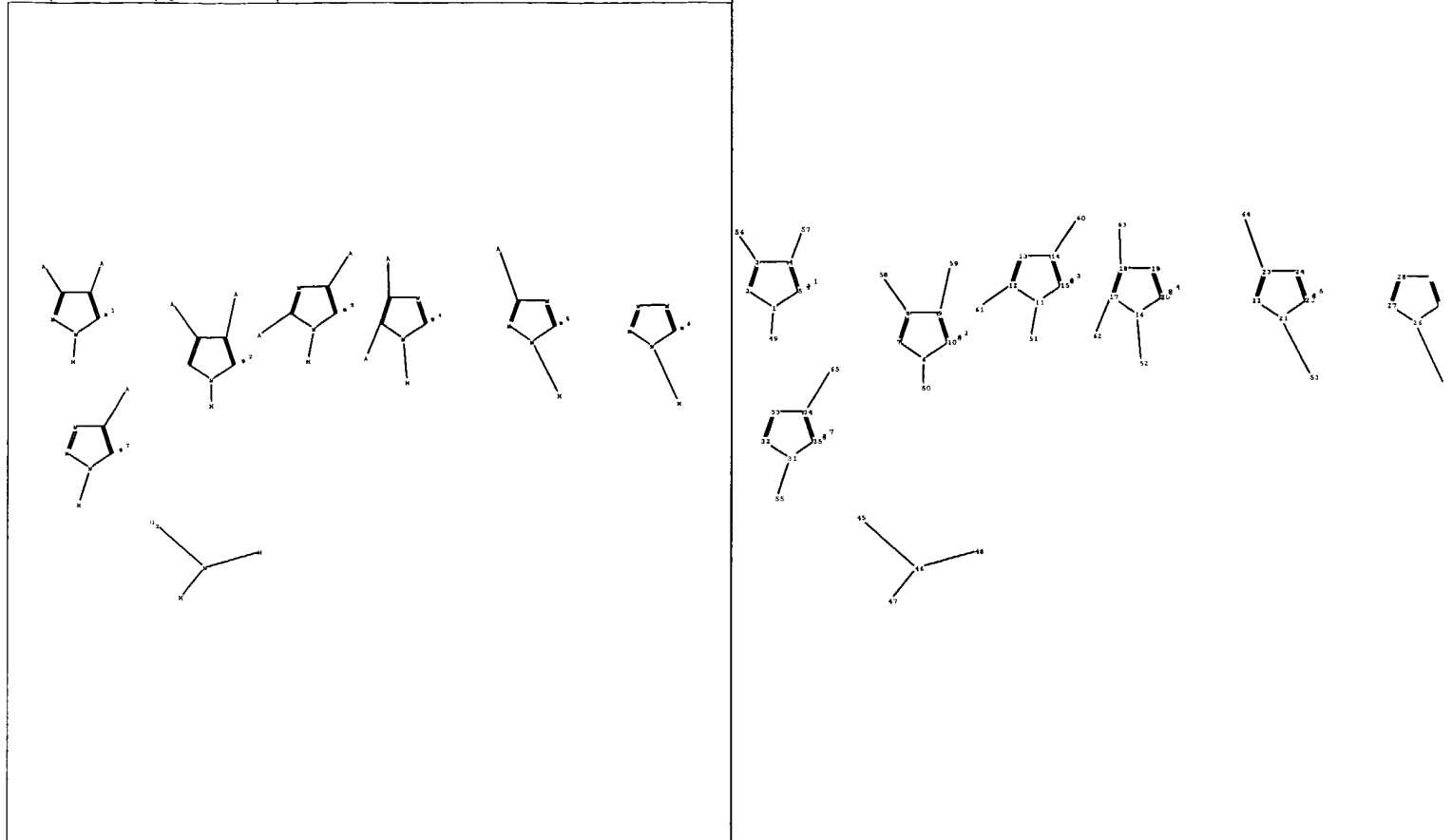
Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom 11:Atom
12:Atom 13:Atom 14:Atom 15:Atom 16:Atom 17:Atom 18:Atom 19:Atom 20:Atom 21:Atom
22:Atom 23:Atom 24:Atom 25:Atom 26:Atom 27:Atom 28:Atom 29:Atom 30:Atom 31:Atom
32:Atom 33:Atom 34:Atom 35:Atom 45:CLASS 46:CLASS 47:CLASS 48:CLASS

fragments assigned product role:

containing 45

C:\stnweb\Queries\6.str



chain nodes :

45 46 47 48 49 50 51 52 53 54 55

ring nodes :

1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16 17 18 19 20 21 22 23 24 25
26 27 28 29 30 31 32 33 34 35

ring/chain nodes :

56 57 58 59 60 61 62 63 64 65

chain bonds :

1-49 3-56 4-57 6-50 8-58 9-59 11-51 12-61 14-60 16-52 17-62 18-63 21-53
23-64 26-54 31-55 34-65 45-46 46-48 46-47

ring bonds :

1-2 1-5 2-3 3-4 4-5 6-7 6-10 7-8 8-9 9-10 11-12 11-15 12-13 13-14 14-15
16-17 16-20 17-18 18-19 19-20 21-22 21-25 22-23 23-24 24-25 26-27 26-30 27-28
28-29 29-30 31-32 31-35 32-33 33-34 34-35

exact/norm bonds :

1-2 1-5 2-3 3-4 3-56 4-5 4-57 6-7 6-10 7-8 8-9 8-58 9-10 9-59 11-12 11-15
12-13 12-61 13-14 14-15 14-60 16-17 16-20 17-18 17-62 18-19 18-63 19-20 21-22
21-25 22-23 23-24 23-64 24-25 26-27 26-30 27-28 28-29 29-30 31-32 31-35 32-33
33-34 34-35 34-65 45-46

exact bonds :

1-49 6-50 11-51 16-52 21-53 26-54 31-55 46-48 46-47

G1:O,S

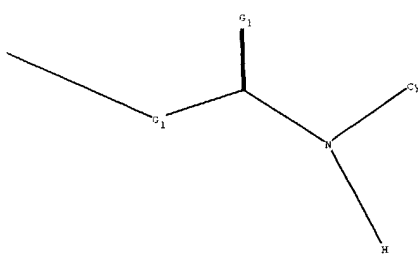
G2:[*1],[*2],[*3],[*4],[*5],[*6],[*7]

Match level :

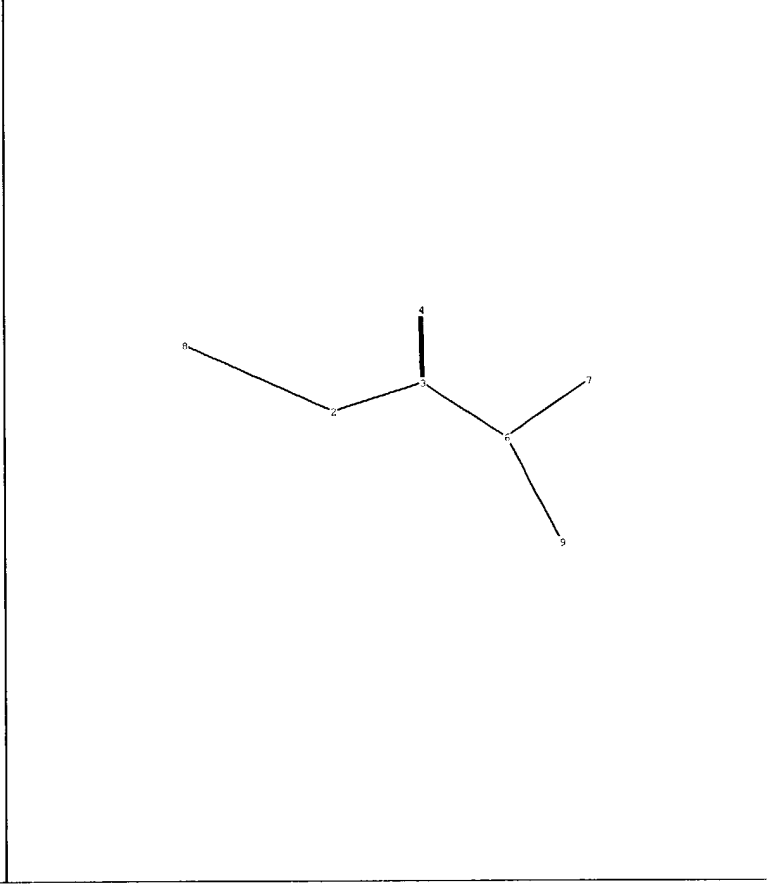
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom 11:Atom
12:Atom 13:Atom 14:Atom 15:Atom 16:Atom 17:Atom 18:Atom 19:Atom 20:Atom 21:Atom
22:Atom 23:Atom 24:Atom 25:Atom 26:Atom 27:Atom 28:Atom 29:Atom 30:Atom 31:Atom
32:Atom 33:Atom 34:Atom 35:Atom 45:CLASS 46:CLASS 47:CLASS 48:CLASS 49:CLASS
50:CLASS 51:CLASS 52:CLASS 53:CLASS 54:CLASS 55:CLASS 56:CLASS 57:CLASS 58:CLASS
59:CLASS 60:CLASS 61:CLASS 62:CLASS 63:CLASS 64:CLASS 65:CLASS

fragments assigned product role:

containing 45



The chemical structure shows a four-carbon chain. The second carbon from the left is bonded to a methyl group (CH₃) and a hydroxyl group (OH). The first carbon is bonded to three hydrogens (CH₃). The third carbon is bonded to two hydrogens (CH₂). The fourth carbon is bonded to three hydrogens (CH₃). The structure is drawn in a skeletal format with explicit labels for the functional groups.



2 3 4 6 7 9

ring/chain nodes :

2-3 2-8 3-4 3-6 6-7 6-9

exact/norm bonds :

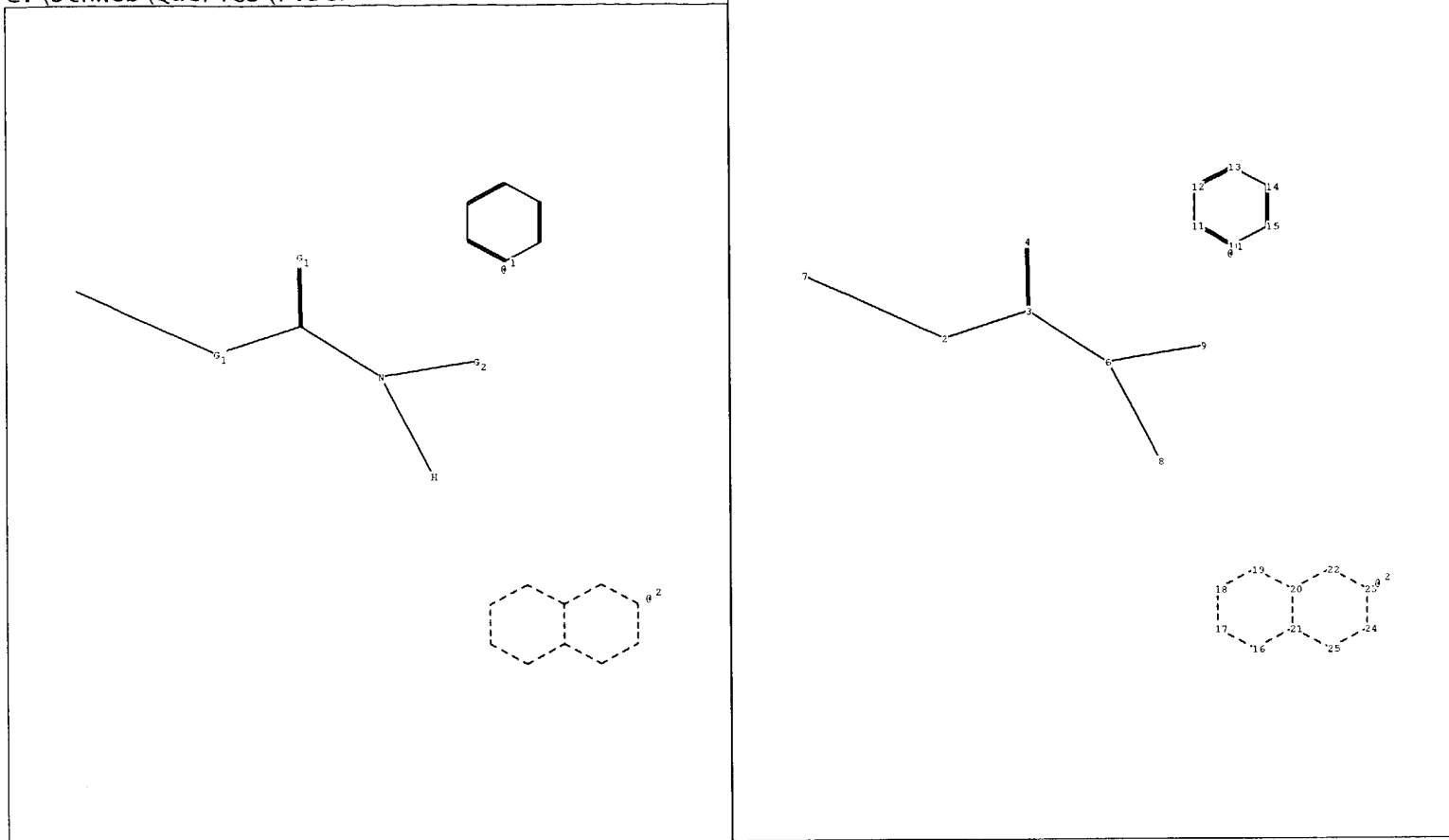
2-3 2-8 3-4 3-6 6-7

exact bonds :

```
2:CLASS 3:CLASS 4:CLASS 6:CLASS 7:Atom 8:CLASS 9:CLASS
```

```
2:CLASS 3:CLASS 4:CLASS 6:CLASS 7:Atom 8:CLASS 9:CLASS
```

c:\stnweb\queries\7.str



chain nodes :

2 3 4 6 8 9

ring nodes :

10 11 12 13 14 15 16 17 18 19 20 21 22 23 24 25

ring/chain nodes :

7

chain bonds :

2-3 2-7 3-4 3-6 6-8 6-9

ring bonds :

10-11 10-15 11-12 12-13 13-14 14-15 16-17 16-21 17-18 18-19 19-20 20-21 20-22
21-25 22-23 23-24 24-25

exact/norm bonds :

2-3 2-7 3-4 3-6 6-9 16-17 16-21 17-18 18-19 19-20 20-21 20-22 21-25 22-23
23-24 24-25

exact bonds :

6-8

normalized bonds :

10-11 10-15 11-12 12-13 13-14 14-15

isolated ring systems :

containing 10 : 16 :

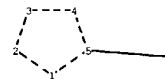
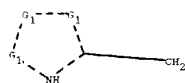
G1:O,S

G2:[*1],[*2]

Match level :

2:CLASS 3:CLASS 4:CLASS 6:CLASS 7:CLASS 8:CLASS 9:Atom 10:Atom 11:Atom 12:Atom
13:Atom 14:Atom 15:Atom 16:Atom 17:Atom 18:Atom 19:Atom 20:Atom 21:Atom 22:Atom
23:Atom 24:Atom 25:Atom

C:\stnweb\Queries\6.str



chain nodes :

8

ring nodes :

1 2 3 4 5

chain bonds :

5-8

ring bonds :

1-2 1-5 2-3 3-4 4-5

exact/norm bonds :

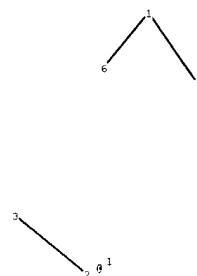
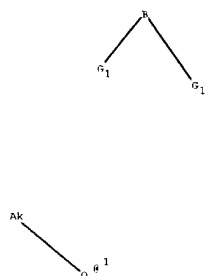
1-2 1-5 2-3 3-4 4-5 5-8

G1:C,N

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 8:CLASS

C:\stnweb\Queries\6.str

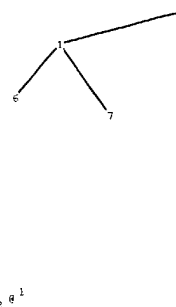
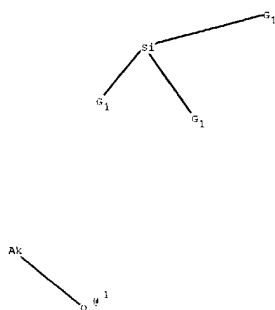


chain nodes :
1 2 3 6 7
chain bonds :
1-6 1-7 2-3
exact/norm bonds :
1-6 1-7 2-3

G1:Ak,OH,X,[*1]

Match level :
1:CLASS 2:CLASS 3:CLASS 6:CLASS 7:CLASS

C:\stnweb\Queries\3.str



chain nodes :

2 3 6 7

ring nodes :

1 9

chain bonds :

1-6 1-7 2-3 9-11

ring bonds :

1-9

exact/norm bonds :

1-6 1-7 1-9 2-3 9-11

G1:Ak,OH,X,[*1]

Match level :

1:CLASS 2:CLASS 3:CLASS 6:CLASS 7:CLASS 9:CLASS